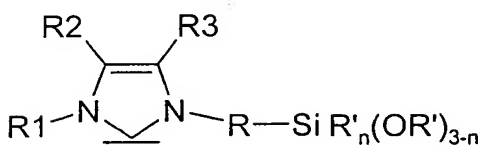
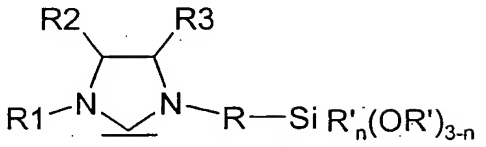
PATENT CLAIMS

1. Compounds of the general formulae (I) and (II)



(I)



(II)

in which

R is A, Ar, A-Ar, A-Ar-A, Het, AHet or AHetA having a total of not more than 30 carbon atoms, where

A is a straight-chain, branched, saturated or mono- or polyunsaturated C_1-C_{20}-alkyl radical, cycloalkyl or cycloalkyl bonded via one or two alkyl group(s) having a total of 4 – 30 carbon atoms, where one CH_2 or CH group both in the alkyl radical and in the cycloalkyl radical may be replaced by N, NH, NA, O and/or S,

Ar is mono- or polysubstituted or unsubstituted phenyl, naphthyl, anthryl or phenanthryl having a total of not more than 20 carbon atoms, where substituents may be A, Hal, OA, CO-AOH, COOH, COOA, COA, OH, CN, CONHA, NO_2, =NH or =O,

Het is a monocyclic or bicyclic, saturated, unsaturated or aromatic heterocyclic radical having from 1 to 4 N, O and/or S atoms, which may be unsubstituted or mono-, di- or trisubstituted by Hal and/or A, OA, CO-AOH, COOH, COOA, COA, OH, CN, CONHA, NO_2, =NH or =O,

R', independently of the position in the molecule, is A, Ar, A-Ar or A-Ar-A having 1 – 12 carbon atoms,

R1 is A, Ar, AAr, AArA, Het, AHet or AHetA having 1 – 18 carbon atoms, in which the radical A which is not bonded to Ar or Het is alkyl or cycloalkyl which is unsubstituted or substituted by one or more groups Z, and Ar is an aromatic hydrocarbon which is unsubstituted or mono- or polysubstituted by a group Z, and Het is a saturated, unsaturated or aromatic heterocyclic radical, which may be mono- or polysubstituted by a group Z, and

R2 and R3, independently of one another, are H, Z, Hal or A, Ar or AAr having 1 – 18 carbon atoms, in which the radical A which is not bonded to Ar or Het is alkyl or cycloalkyl which is unsubstituted or substituted by one or more groups Z, and Ar is an aromatic hydrocarbon which is unsubstituted or mono- or polysubstituted by a group Z,

where

Hal is F, Cl, Br or I,

Z, independently of the position in R1, R2 and R3, is an N, P, O or S atom-containing functional group, A or Ar, and

n is 0, 1 or 2.

2. Compounds according to Claim 1 of the general formulae (I) and (II), in which

R is A, Ar, A-Ar, A-Ar-A, Het, AHet or AHetA having a total of not more than 20 carbon atoms,

R', independently of the position in the molecule, is a straight-chain, branched, saturated, mono- or polyunsaturated C_1-C_7-alkyl radical,

R1 is A, Ar, AAr, AArA, Het, AHet or AHetA having 1 – 18 carbon atoms, in which the radical A which is not bonded to Ar or Het is alkyl or cycloalkyl which is unsubstituted or substituted by one or more groups Z, and Ar is an aromatic hydrocarbon which is unsubstituted or mono- or polysubstituted by a group Z, and Het is a saturated, unsaturated or aromatic heterocyclic radical, which may be mono- or polysubstituted by a group Z, and

R2 and R3, independently of one another, are H, Cl, Br or a straight-chain, branched, saturated, mono- or polyunsaturated C_1-C_7-alkyl radical,

Z is A,

and

n is 0,

and A, Ar and Het are as defined in Claim 1.

3. Compounds according to Claim 1 of the general formulae (I) and (II), in which

R is A, Ar, A-Ar or A-Ar-A having a total of not more than 20 carbon atoms, where
A is a straight-chain or branched, saturated C_1-C_{12}-alkyl radical, cycloalkyl having 3 – 10 carbon atoms or C_4-C_{20}-cycloalkyl bonded via one or two alkyl group(s),
Ar is phenyl which is mono- or polysubstituted or unsubstituted, where substituents can adopt the meanings of A, and R has a total of not more than 20 carbon atoms,

R', independently of the position in the molecule, is a straight-chain, branched, saturated C_1-C_7-alkyl radical,

R1 is A having the meaning of cycloalkyl which is unsubstituted or substituted by one or more groups Z,
or
Ar an aromatic hydrocarbon which is unsubstituted or substituted by Z = A,

R2 and R3, independently of one another, are H or a straight-chain, branched, saturated C_1-C_7-alkyl radical,

Z is A,

and

n is 0,

and A and Ar are as defined in Claim 1.

4. Compounds according to Claim 1 of the general formulae (I) and (II), in which

R', independently of the position in the molecule, is
methyl, ethyl, propyl, isopropyl, butyl, isobutyl, sec- or tert-butyl, pentyl, 1-, 2- or 3-methylbutyl (-C_5H_{10}-), 1,1-, 1,2- or 2,2-dimethylpropyl (-C_5H_{10}-), 1-ethylpropyl (-C_5H_{10}-), hexyl (-C_6H_{12}-), 1-, 2-, 3- or 4-methylpentyl (-C_6H_{12}-), 1,1-, 1,2-, 1,3-, 2,2-, 2,3- or 3,3-dimethylbutyl (-C_6H_{12}-), 1- or 2-ethylbutyl (-C_6H_{12}-), 1-ethyl-1-methylpropyl (-C_6H_{12}-), 1-ethyl-2-methylpropyl (-C_6H_{12}-), 1,1,2- or 1,2,2-trimethylpropyl (-C_6H_{12}-), heptyl or octyl.

5. Compounds according to Claim 1 of the general formulae (I) and (II), in which

R is A, Ar or A-Ar,
where

A is a straight-chain, saturated C_1-C_{12}-alkyl radical or C_3-C_9-cycloalkyl, or
Ar is phenyl, unsubstituted or mono- or polysubstituted by Z = A,
R', independently of the position in the molecule, is a straight-chain or branched, saturated C_1-C_4-alkyl radical,
R1 is A having the meaning of cycloalkyl,
or
Ar is an aromatic hydrocarbon which is unsubstituted or mono- or polysubstituted by Z = A,
R2 and R3 are H,
and
n is 0,
and A and Ar are as defined in Claim 1.

6. Compounds according to Claim 1 of the general formulae (I) and (II), in which
R is methyl, ethyl, propyl, isopropyl, butyl, isobutyl, sec- or tert-butyl, 1,2-cyclopropyl, 1,2- or 1,3-cyclobutyl, 1,2- or 1,3-cyclopentyl, 1,2-, 1,3- or 1,4-cyclohexyl, furthermore 1,2-, 1,3- or 1,4-cycloheptyl, methylcyclopentyl, methylcyclohexyl, phenyl, benzyl (-$CH_2C_6H_4$-), tolyl (-$C_6H_3(CH_3)$-), -$C_6H_2(CH_3)_2$-, -$CH_2C_6H_2(CH_3)_2$-, -$CH_2C_6H_4CH_2$-, -$CH_2C_6H_2(CH_3)_2CH_2$-, trimethylphenyl or naphthyl,
R' is methyl, ethyl, propyl, isopropyl, butyl, isobutyl, sec- or tert-butyl,
R3 is cyclopropyl, cyclobutyl, cyclopentyl, cyclohexyl, methylcyclopentyl, cycloheptyl, methylcyclohexyl, cyclooctyl, furanyl, phenyl, benzyl, tolyl, trimethylphenyl, 2,4,6-methylphenyl (mesityl), triisopropylphenyl or naphthyl,
R1, R2 and R4 are H, methyl or ethyl,
n is 0.

7. 1-[3-(triethoxysilyl)ethyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[3-(trimethoxysilyl)ethyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[3-(triethoxysilyl)propyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene

1-[3-(trimethoxysilyl)propyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[3-(triethoxysilyl)butyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[3-(trimethoxysilyl)butyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[3-(triethoxysilyl)ethyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)ethyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(triethoxysilyl)propyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)propyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(triethoxysilyl)butyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)butyl]-3-(mesityl)imidazol-2-ylidene
1-[3-(triethoxysilyl)ethyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)ethyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)propyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)propyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)butyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)butyl]-3-(phenyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)ethyl]-3-(cyclohexyl)imidazol-2-ylidene
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1-[3-(triethoxysilyl)propyl]-3-(cyclohexyl)imidazol-2-ylidene
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1-[3-(triethoxysilyl)butyl]-3-(cyclohexyl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)butyl]-3-(cyclohexyl)imidazol-2-ylidene
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1-[3-(trimethoxysilyl)ethyl]-3-(t-butyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)propyl]-3-(t-butyl)imidazol-2-ylidene
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1-[3-(triethoxysilyl)butyl]-3-(t-butyl)imidazol-2-ylidene
1-[3-(trimethoxysilyl)butyl]-3-(t-butyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)ethyl]-3-(i-propyl)imidazol-2-ylidene
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1-[3-(trimethoxysilyl)ethyl]-3-(methyl)imidazol-2-ylidene
1-[3-(triethoxysilyl)propyl]-3-(methyl)imidazol-2-ylidene

1-[3-(trimethoxysilyl)propyl]-3-(methyl)imidazol-2-ylidene
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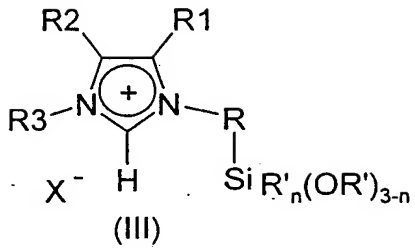
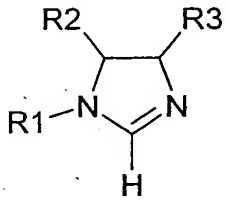
1-[3-(trimethoxysilyl)butyl]-3-(methyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(mesityl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(mesityl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(cyclohexyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(cyclohexyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(methyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(methyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(phenyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(phenyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(i-propyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(i-propyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-(t-butyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-(t-butyl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)benzyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[4-(triethoxysilyl)benzyl]-3-[2,4-(di-i-propyl)phenyl]imidazol-2-ylidene
1-[4-(trimethoxysilyl)-2,4-(dimethyl)phenyl]-3-(mesityl)imidazol-2-ylidene
1-[4-(triethoxysilyl)-2,4-(dimethyl)phenyl]-3-(mesityl)imidazol-2-ylidene
1-[4-(trimethoxysilyl)-2,4-(dimethyl)phenyl]-3-(cyclohexyl)imidazol-2-ylidene
1-[4-(triethoxysilyl)-2,4-(dimethyl)phenyl]-3-(cyclohexyl)imidazol-2-ylidene
as compounds according to Claim 1.

8. Process for the preparation of compounds of the general formulae (I) and (II), characterised in that a substituted imidazole of the general formula (III)



(III)

or a substituted 4,5-dihydroimidazole of the general formula (IV)

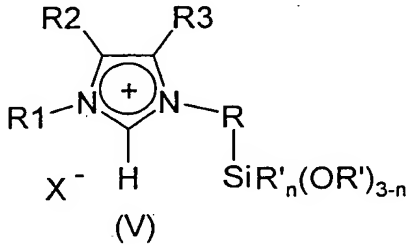


(IV)

is reacted with a chlorine-, bromine- or iodine-containing alkoxysilane of the general formula

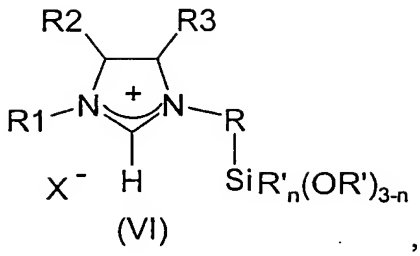
$$Hal\text{-}R\text{-}SiR'_n(OR')_{3-n}$$

optionally in an inert, aprotic, organic solvent, to give alkoxysilyl-functionalised imidazolium salts of the general formula (V)



(V)

or alkoxysilyl-functionalised 4,5-dihydroimidazolium salts of the general formula (VI) respectively



(VI)

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where, in the general formulae, R, R', R1, R2 and R3 can adopt the meanings of the preceding claims, and X^- can be an anion from the group consisting of F^-, Cl^-, Br^- and I^-,
and
the resultant compounds of the general formula (V) or (VI) respectively, either directly in the resultant reaction mixture or after separation and, if necessary, purification, are reacted with a base selected from the group consisting of metal alkoxides (MOR), metal hydrides (MH), metal amides (MNH_2) and/or ammonia in an anhydrous, inert, aprotic, organic solvent which has, if appropriate, already been added in order to carry out the previous reaction, to give the carbenes of the general formulae (I) and (II) respectively.

9. Process according to Claim 8, characterised in that, for the isolation and purification of the carbenes of the general formulae (I) and (II), after any solid by-products that have formed have been removed by filtration, the volatile constituents are separated off in a high vacuum, and the crude product is purified by extraction and, if desired, by crystallisation.

10. Process according to Claim 8 or 9, characterised in that the compounds of the general formulae (V) and (VI) are reacted with a metal alkoxide MOR, metal hydride MH or with NH_3/NaH as base to give a carbene of the general formulae (I) and (II) respectively, where an inert solvent selected from the group consisting of hexane, benzene, toluene and xylene; petroleum ether; ethers, such as diethyl ether, diisopropyl ether, tetrahydrofuran (THF) and dioxane; glycol ethers, such as ethylene glycol dimethyl ether (diglyme); ketones, such as acetone and butanone; esters, such as ethyl acetate, and mixtures of the said solvents, is used.

11. Process according to one or more of Claims 8 to 10, characterised in that the compounds of the general formulae (V) and (VI) are reacted with a metal alkoxide MOR or metal hydride MH as base in a solvent selected from the group consisting of hydrocarbons, such as hexane, benzene, toluene and xylene; petroleum ether, ethers, such as diethyl ether, diisopropyl ether, tetrahydrofuran (THF) and dioxane.

12. Process according to one or more of Claims 8 to 11, characterised in that the compounds of the general formulae (V) and (VI) are reacted with KO^tBu or KH as base to give carbenes of the general formulae (I) and (II) respectively.

13. Process according to one or more of Claims 8 to 12, characterised in that, for the preparation of the carbenes of the general formulae (I) and (II), the starting materials imidazolium salt [(V) or (VI)] and base are employed in a stoichiometric ratio in a range between 1:1 and 1:10, preferably between 1:1 and 1:3 and particularly preferably between 1:1 and 1:1.2, and the reaction is carried out under a protective-gas atmosphere consisting of a gas selected from the group consisting of nitrogen and argon, where the temperature is held in a range from -78°C to +100°C, preferably from -40°C to +60°C and very preferably between 0°C and 30°C.

14. Process according to one or more of Claims 8 to 13, characterised in that the reaction of the starting materials imidazolium salt [(V) or (VI)] with a base to give carbenes of the general formulae (I) and (II) respectively is carried out within a reaction time of from one minute to 6 hours, preferably from five minutes to 2 hours and very preferably within from 10 minutes to 1 hour.

15. Use of compounds of the general formulae (I) and (II) as starting material for the preparation of immobilised N-heterocyclic carbenes and N-heterocyclic carbene complexes.

16. Use of compounds of the general formulae (I) and (II) as complex ligands for the preparation of immobilisable N-heterocyclic carbene

complexes containing main-group metal atoms, rare-earth metal atoms and transition-metal atoms.

17. Use of compounds of the general formulae (I) and (II) as starting material for the preparation of immobilisable catalysts or immobilised N-heterocyclic carbene catalyst ligands.

18. Use of compounds of the general formulae (I) and (II) as components or catalysts in organic or organometallic and transition metal-catalysed reactions.

19. Use of compounds of the general formulae (I) and (II) as catalyst ligands in catalytic reactions, preferably in C-C coupling reactions, oligomerisations, hydrogenations, hydroformylations, aminations, oxidations and reductions.

20. Use of compounds of the general formulae (I) and (II) as reaction media in organic or organometallic and transition metal-catalysed reactions.

21. Use of compounds of the general formulae (I) and (II) as starting materials for immobilised reaction media.

22. Use of compounds of the general formulae (I) and (II) as medium for the purification of reaction products (scavenger function).